The Lie Algebra Structure and Nonlinear Controllability of Spin Systems

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Abstract

In this paper, we study the controllability properties and the Lie algebra structure of networks of particles with spin immersed in an electro-magnetic field. We relate the Lie algebra structure to the properties of a graph whose nodes represent the particles and an edge connects two nodes if and only if the interaction between the two corresponding particles is active. For networks with different gyromagnetic ratios, we provide a necessary and sufficient condition of controllability in terms of the properties of the above mentioned graph and describe the Lie algebra structure in every case. For these systems all the controllability notions, including the possibility of driving the evolution operator and/or the state, are equivalent. For general networks (with possibly equal gyromagnetic ratios), we give a sufficient condition of controllability. A general form of interaction among the particles is assumed which includes both Ising and Heisenberg models as special cases.

Assuming Heisenberg interaction we provide an analysis of low dimensional cases (number of particles less then or equal to three) which include necessary and sufficient controllability conditions as well as a study of their Lie algebra structure. This also, provides an example of quantum mechanical systems where controllability of the state is verified while controllability of the evolution operator is not.

Keywords: Controllability of Quantum Mechanical Systems, Lie Algebra Structure, Particles with Spin.

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1 Introduction

The controllability of multilevel quantum mechanical systems described by bilinear models can be investigated using results on the controllability of bilinear systems varying on Lie groups [11], [18]. In particular, general results established in [12] can be applied to this case leading to the calculation of the Lie algebra generated by the Hamiltonian of the system and the verification of a rank condition. The determination of this Lie algebra for *classes* of quantum systems is a problem of both fundamental and practical importance in the theory of quantum control. In fact, it gives the set of states that can be obtained by driving the system opportunely and letting it evolve for an appropriate amount of time. Previous work in this direction, for various classes of quantum systems, was done in [4], [21].

In this paper, we analyze the Lie algebra structure and give conditions of controllability for a network of interacting spin $\frac{1}{2}$ particles in a driving electro-magnetic field. Spin $\frac{1}{2}$ particles are of great interest because they can be used as elementary pieces of information (quantum bits) in quantum information theory [9]. These systems can be driven with techniques of Nuclear Magnetic Resonance [5]. A study of their controllability properties gives information on what state transfers can be obtained with a given physical set-up. A previous study on the controllability of this system was carried out in [14], [22]. Results on the controllability of systems of one and two spin $\frac{1}{2}$ particles can be found in [6], [13].

In the present paper we relate the Lie algebra structure of a network of spin $\frac{1}{2}$ particles to the properties of a graph whose nodes represent the particles and whose edges represent the interaction between the particles. We analyze first the case of networks with particles with different gyromagnetic ratios. For these systems we give a necessary and sufficient condition of controllability in terms of connectedness of the associated graph and describe the Lie algebra structure in every case. It will follow from this analysis that all the controllability conditions are equivalent for this class of systems. In particular it is possible to drive the *state* of the system to any configuration if and only if it is possible to drive the *evolution operator* to any unitary operator. We consider then systems with possibly equal gyromagnetic ratio and give a sufficient condition of controllability in this case. Complete results including necessary and sufficient conditions of various types of controllability are obtained for low dimensional cases, namely for a number of particles ≤ 3. These cases are the most common in practical applications. We assume here (for the case number of particles $= 3$) an Heisenberg model for the interaction between particles. In this analysis we also display an example of a model which is controllable in the state but not controllable in the evolution operator.

The paper is organized as follows. In Section 2 we review general notions of controllability for quantum mechanical systems. We recall some results proved in [1] about the relation among different notions of controllability as well as some of the results of [11], [12], [18] about controllability of quantum systems. In Section 3, we describe the general model of systems of n interacting spin $\frac{1}{2}$ particles and define some notations used in the paper. In Section 4 we prove a Lemma which describes a particular subalgebra of the total Lie algebra, that we call the 'Control subalgebra'. This will play an important role in the following development. In Section 5 we study the Lie algebra structure associated to the model described in Section 3 assuming that all the particles have different gyromagnetic ratios. In Section 6, we remove this assumption and prove a general sufficient condition of controllability. We study low dimensional cases in Section 7 and give some conclusions in Section 8.

2 Controllability of Quantum Mechanical Systems

In many physical situations the dynamics of a multilevel quantum system can be described by Schrödinger equation in the form, [7], [18],

$$|\dot{\psi}> = H|\psi> = (A + \sum_{i=1}^{m} B_i u_i(t))|\psi>, \tag{1}$$

where $|\psi>$[1] is the state vector varying on the complex sphere $S_{\mathbb{C}}^{n-1}$ defined as the set of n-ples of complex numbers $x_j + iy_j$, $j = 1, ..., n$, with $\sum_{j=1}^{n} x_j^2 + y_j^2 = 1$. H is called the Hamiltonian of the system. The matrices A, $B_1, ..., B_m$ are in the Lie algebra of *skew-Hermitian* matrices of dimension n, $u(n)$. If A and B_i, $i = 1, ..., m$, have zero trace, they are in the Lie algebra of skew Hermitian matrices with zero trace $su(n)$[2]. The functions $u_i(t)$, $i = 1, 2, ..., m$, are time varying components of electro-magnetic fields that play the role of *controls*. They are assumed to be piecewise continuous, however the considerations in the following would not change had we considered other classes of controls such as piecewise constant or bang bang controls.

The solution of (1) at time t, $|\psi(t)>$ with initial condition $|\psi_0>$ is given by

$$|\psi(t)>= X(t)|\psi_0>, \tag{2}$$

where $X(t)$ is the solution at time t of the equation

$$\dot{X}(t) = (A + \sum_{i=1}^{m} B_i u_i(t))X(t), \tag{3}$$

with initial condition $X(0) = I_{n\times n}$. The solution $X(t)$ varies on the Lie group of unitary matrices $U(n)$ or the Lie group of special unitary matrices $SU(n)$ if the matrices A and B_i in (3) have zero trace.

Various notions of controllability can be defined for system (1). In particular, we will consider the following three.

- System (1) is said to be *Operator Controllable* if it is possible to drive X in (3) to any value in $U(n)$ (or $SU(n)$).

[1]We use Dirac notation $|\psi>$ to denote a vector on $\mathbb{C}^n$ of length 1, and $<\psi| := |\psi>^*$ where * denotes transposed conjugate.

[2]Since trace of A and B_i, $i = 1, 2, ..., m$, only introduce a phase factor in the solution of (1), and states that differ by a phase factor are physically indistinguishable, it is possible to transform the equation (1) into an equivalent one of the same form where the matrices A and B_i, $i = 1, ..., m$, are skew-Hermitian and with zero trace, namely they are in $su(n)$.

- System (1) is *State Controllable* if it is possible to drive the state $|\psi>$ to any value on the complex sphere S_C^{n-1}, for any given initial condition.

- System (1) is said to be *Equivalent State Controllable* if it is possible to drive the state $|\psi>$ to any value on the complex sphere modulo a phase factor $e^{i\phi}$, $\phi \in \mathbf{R}$.

From a physics point of view, equivalent state controllability is equivalent to state controllability since states that differ only by a phase factor are physically indistinguishable.

From the expression (2) for $|\psi>$, it is clear that state controllability is related to the possibility of driving X to a subset of $SU(n)$ or $U(n)$ which is transitive on the complex sphere. Transitivity of transformation groups on spheres was studied in [2], [16], [17], [20] and the necessary connections for application to quantum mechanical systems where made in [1]. In the following theorem, we summarize some of the results of [1] that will be used in the following. Part 2) of the Theorem was proved in [11], [12], [18]. Here and in the following we will denote by $\mathcal{L}$ the Lie algebra generated by $A, B_1, \ldots, B_m$ in (1).

Theorem 1

1. *A quantum mechanical system (1) is state controllable if and only if it is equivalent state controllable. Both these conditions are implied by operator controllability.*

2. *The system is operator controllable if and only if the Lie algebra $\mathcal{L}$ generated by the matrices $A, B_1, ..., B_m$ is $u(n)$ or $su(n)$.*

3. *The system is state controllable if and only if $\mathcal{L}$ is $su(n)$ or $u(n)$, or, in the case of n even, isomorphic to $sp(\frac{n}{2})$*[3].

4. *Consider the $n \times n$ matrix with i in the position $(1,1)$ and zero everywhere else. Call this matrix D. Let $\mathcal{D}$ be the subalgebra of $\mathcal{L}$ of matrices that commute with D. Then, the system is state controllable if and only if $\dim \mathcal{L} - \dim \mathcal{D} = 2n-2$.*

5. *Assume n even. There is no subalgebra of $su(n)$ which contains properly any subalgebra isomorphic to $sp(\frac{n}{2})$ other than $su(n)$ itself.*

Because of the equivalence between state controllability and equivalent state controllability, in the sequel we will only refer to the two notions of state controllability and operator controllability. Controllability notions in a density matrix description of quantum dynamics were considered in [1].

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[3] Recall the Lie algebra of symplectic matrices $sp(k)$ is the Lie algebra of matrices X in $su(2k)$ satisfying $XJ + JX^T = 0$, with J given by $J = \begin{pmatrix} 0 & I_{k\times k} \\ -I_{k\times k} & 0 \end{pmatrix}$

3 Model of interacting spin $\frac{1}{2}$ particles

From this point on, we will denote by n (which in the previous section denoted the dimension of a general quantum system) the number of spin $\frac{1}{2}$ particles in a network. The state dimension of this system is 2^n.

To define the model we will study, we first need to recall some definitions. The following three matrices in $su(2)$ are called *Pauli matrices* (see e.g. [19]):

$$\sigma_x := \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z := \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4}$$

The Pauli matrices satisfy the fundamental commutation relations

$$[\sigma_x, \sigma_y] = i\sigma_z; \qquad [\sigma_y, \sigma_z] = i\sigma_x; \qquad [\sigma_z, \sigma_x] = i\sigma_y. \tag{5}$$

It is known that the matrices $i\sigma_x$, $i\sigma_y$, $i\sigma_z$ form a basis in $su(2)$. Moreover, the set of matrices $i(\sigma_1 \otimes \sigma_2 \otimes \cdots \otimes \sigma_n)$, where σ_j, $j = 1, ...n$, is equal to one of the Pauli matrices or the 2×2 identity $I_{2\times 2}$, without $i(I_{2\times 2} \otimes I_{2\times 2} \otimes \cdots \otimes I_{2\times 2})$, form a basis in $su(2^n)$. (Here $\otimes$ indicates the Kronecker product for matrices.)

In the following, we will use the notation I_{kx} for the Kronecker product

$$I_{kx} := \sigma_1 \otimes \sigma_2 \otimes \cdots \otimes \sigma_n, \tag{6}$$

where all the the elements σ_j, $j = 1, ..., n$ are equal to the 2×2 identity matrix, except the $k-$th element which is equal to σ_x. More in general, we will use the notation $I_{k_1 l_1, k_2 l_2, ..., k_r l_r}$, with $1 \leq k_1 < k_2 < \cdots < k_r \leq n$ and $l_j = x, y$ or z, $j = 1, ..., r$, for a Kronecker product of the form (6) where all the σ_j are equal to the identity $I_{2\times 2}$ except the ones in the k_j-th positions which are equal to the Pauli matrices σ_{l_j}. The matrices so defined (excluding the identity matrix) span $su(2^n)$. Some elementary properties of the commutators of the matrices just defined that will be used in the following are collected in Appendix A.

The Hamiltonian of the system of n interacting spin $\frac{1}{2}$ particles in a driving electromagnetic field is given in the form [3]:

$$H = H_0 + H_I. \tag{7}$$

Here H_0, which denotes the *internal (or unperturbed) Hamiltonian*, is given by

$$H_0 := \sum_{k<l}^{n} (M_{kl} I_{kx,lx} + N_{kl} I_{ky,ly} + P_{kl} I_{kz,lz}), \tag{8}$$

where M_{kl}, N_{kl}, P_{kl} are the coupling constants between particle k and particle l. This general model of the interaction between different particles includes as special cases both the Ising and the Heisenberg model ([15], pg. 46). The term H_I, *Control Hamiltonian*, is given by

$$H_I := (\sum_{k=1}^{n} \gamma_k I_{kx}) u_x(t) + (\sum_{k=1}^{n} \gamma_k I_{ky}) u_y(t) + (\sum_{k=1}^{n} \gamma_k I_{kz}) u_z(t), \tag{9}$$

where u_x, u_y and u_z are the x, y and z components of the electro-magnetic field and γ_j, $j=1,2,...$, is the gyromagnetic ratio of the j-th particle. In general, we assume that we are able to vary all the three components of the magnetic field for control (cfr. Remark 5.2). Schrödinger equation (3) for the evolution matrix X has the form,

$$\dot{X} = AX + B_x X u_x + B_y X u_y + B_z X u_z, \tag{10}$$

with

$$A := -i \sum_{k<l,k,l=1}^{n} (M_{kl} I_{kx,lx} + N_{kl} I_{ky,ly} + P_{kl} I_{kz,lz}),$$

and

$$B_v := -i(\sum_{k=1}^{n} \gamma_k I_{kv}), \quad \text{with} \;\; v = x,\, y, \;\; \text{or} \;\; z.$$

It is clear that the controllability properties of this class of systems only depends on the parameters M_{kl}, N_{kl}, P_{kl} and γ_k. Our goal in the next sections is to characterize the structure of the Lie algebra generated by A and B_x, B_y, B_z, $\mathcal{L}$, in terms of these parameters. The network of spin particles can be represented by a graph whose nodes represent the particles and are labeled by their gyromagnetic ratios and an edge connects the nodes corresponding to particles k and l if and only if at least one of the coupling constants M_{kl}, N_{kl}, P_{kl} is different from zero. In this case, the edge is labeled by the triple $\{M_{kl}, N_{kl}, P_{kl}\}$. It is our goal, in the next sections, to relate the properties of the Lie algebra $\mathcal{L}$, generated by A, B_x, B_y and B_z to the properties of this graph. In the following, we denote this graph by $\mathcal{G}\nabla$.

We define an ordering on the n particles so that the first n_1 have the same gyromagnetic ratio γ_1, the next n_2 particles all have gyromagnetic ratio γ_2, with $\gamma_2 \neq \gamma_1$, and so on up to the $r-$th set of n_r particles with gyromagnetic ratio γ_r, with $\gamma_j \neq \gamma_k$ when $j \neq k$ and $n_1 + n_2 + n_3 + \cdots + n_r = n$. We shall denote the first set of particles by S_1^0, the second one by S_2^0, and so on up to the $r-$th, S_r^0. We also define, for $j = 1, 2, ..., r$, $v = x, y, z$

$$\tilde{I}_{jv} := \sum_{h \in S_j^0} I_{hv}, \tag{11}$$

and we have

$$B_v := -i \sum_{j=1}^{r} \gamma_j \tilde{I}_{jv}.$$

For a given system, we shall call the *Control Subalgebra* of $\mathcal{L}$, the subalgebra generated by the matrices B_x, B_y and B_z. We shall denote the control subalgebra by $\mathcal{B}$.

4 Characterization of the Control Subalgebra

The following lemma shows that the control subalgebra $\mathcal{B}$ of a spin system is the direct sum of r subalgebras isomorphic to $su(2)$.

Lemma 4.1 Assume we are given a model as in (10), and let $\gamma_1, \dots, \gamma_r$ be the different values for the gyromagnetic ratios. Assume that to each value γ_j correspond n_j particles in the set S_j^0, $j = 1, \dots, r$, then the matrices B_x, B_y and B_z generate the following Lie algebra:

$$\mathcal{B} = \mathcal{B}_x \oplus \mathcal{B}_y \oplus \mathcal{B}_z, \tag{12}$$

with:

$$\mathcal{B}_x = span_{j=1,\dots,r}\{i\tilde{I}_{jx}\}, \tag{13}$$
$$\mathcal{B}_y = span_{j=1,\dots,r}\{i\tilde{I}_{jy}\}, \tag{14}$$
$$\mathcal{B}_z = span_{j=1,\dots,r}\{i\tilde{I}_{jz}\}. \tag{15}$$

Moreover, we have:

$$[\mathcal{B}_x, \mathcal{B}_y] = \mathcal{B}_z, \qquad [\mathcal{B}_y, \mathcal{B}_z] = \mathcal{B}_x, \qquad [\mathcal{B}_z, \mathcal{B}_x] = \mathcal{B}_y. \tag{16}$$

Proof. First, notice that $\tilde{I}_{j(x,y,z)}$ satisfy the commutation relations

$$[\tilde{I}_{jx}, \tilde{I}_{ky}] = i\delta_{jk}\tilde{I}_{jz}, \quad [\tilde{I}_{jy}, \tilde{I}_{kz}] = i\delta_{jk}\tilde{I}_{jx}, \quad [\tilde{I}_{jz}, \tilde{I}_{kx}] = i\delta_{jk}\tilde{I}_{jy}, \tag{17}$$

where we used the Kronecker symbol δ_{jk}. We proceed by induction on $r \geq 1$. If $r = 1$, then we have, for $v \in \{x,\ y\ z\}$:

$$B_v = -i\tilde{I}_{1v},$$

thus (12)-(16) follow immediately from the basic commutation relations (17).

To prove the inductive step, we first show, again by induction on $r \geq 1$ that:

$$\begin{array}{rcl} [B_x, B_y] & = & -i\sum_{j=1}^r \gamma_j^2 \tilde{I}_{jz}, \\ [B_y, B_z] & = & -i\sum_{j=1}^r \gamma_j^2 \tilde{I}_{jx}, \\ [B_z, B_x] & = & -i\sum_{j=1}^r \gamma_j^2 \tilde{I}_{jy}. \end{array} \tag{18}$$

We will prove only the first of the previous equalities, since the other ones may be obtained in the same way. If $r = 1$, then

$$[B_x, B_y] = -\gamma_1^2[\tilde{I}_{1x}, \tilde{I}_{1y}] = -i\gamma_1^2\tilde{I}_{1z},$$

where to get the last equality we have used (17). Now let $r > 1$:

$$[B_x, B_y] = -[\sum_{j=1}^r \gamma_j\tilde{I}_{jx}, \sum_{j=1}^r \gamma_j\tilde{I}_{jy}] =$$

$$-\left([\sum_{j=1}^{r-1} \gamma_j\tilde{I}_{jx}, \sum_{j=1}^{r-1} \gamma_j\tilde{I}_{jy}] + \sum_{j=1}^{r-1}[\gamma_j\tilde{I}_{jx}, \gamma_r\tilde{I}_{ry}] + \sum_{j=1}^{r-1}[\gamma_r\tilde{I}_{rx}, \gamma_j\tilde{I}_{jy}] + [\gamma_r\tilde{I}_{rx}, \gamma_r\tilde{I}_{ry}]\right).$$

By the inductive assumption, we have:

$$[\sum_{j=1}^{r-1} \gamma_j\tilde{I}_{jx}, \sum_{j=1}^{r-1} \gamma_j\tilde{I}_{jy}] = i\sum_{j=1}^{r-1} \gamma_j^2\tilde{I}_{jz}. \tag{19}$$

Using (17), we obtain, for $j < r$,

$$\begin{aligned} [\gamma_j \tilde{I}_{jx}, \gamma_r \tilde{I}_{ry}] = 0, \\ [\gamma_r \tilde{I}_{rx}, \gamma_j \tilde{I}_{jy}] = 0, \end{aligned} \tag{20}$$

and

$$[\gamma_r \tilde{I}_{rx}, \gamma_r \tilde{I}_{ry}] = i\gamma_r^2 \tilde{I}_{rz}. \tag{21}$$

Now putting together equations (19), (20) and (21), we get:

$$[B_x, B_y] \;=\; -i\sum_{j=1}^{r} \gamma_j^2 \tilde{I}_{jz},$$

as desired. Thus, we have proved (18).

Now notice that, for example, $[B_y, B_z]$ has the same form as B_x except that the γ_j's have been replaced by γ_j^2, therefore, using the same arguments as above one may show that:

$$[[B_y, B_z], B_y] = -i\sum_{j=1}^{r} \gamma_j^3 \tilde{I}_{jz}. \tag{22}$$

More in general, considering the Lie bracket between $F_x := -i\sum_{j=1}^{r} \gamma_j^k \tilde{I}_{jx}$, and $G_y := -i\sum_{j=1}^{r} \gamma_j^l \tilde{I}_{jy}$, we get $S := -i\sum_{j=1}^{r} \gamma_j^{k+l} \tilde{I}_{jz}$. Proceeding this way, we obtain all the matrices

$$i\sum_{j=1}^{r} \gamma_j^l \tilde{I}_{jx}, \tag{23}$$

$$i\sum_{j=1}^{r} \gamma_j^l \tilde{I}_{jy}, \tag{24}$$

and

$$i\sum_{j=1}^{r} \gamma_j^l \tilde{I}_{jz}, \tag{25}$$

$l = 1, ..., r$. The matrices in (23) form a basis in $\mathcal{B}_x$ since the $\tilde{I}_{jx}$ do and the linear transformation in (23) is nonsingular. In fact, the corresponding determinant is a Vandermonde determinant which is different from zero because all the γ_j's are different from each other. The same is true for the elements in (24) and (25) which form a basis in $\mathcal{B}_y$ and $\mathcal{B}_z$, respectively. Finally, the commutation relations (16) follow immediately from (17). $\square$

Notice that it follows from (17) and (5) that the subalgebras spanned by $\tilde{I}_{j(x,y,z)}$ are each isomorphic to $su(2)$ and they commute with each other. For a given j, the Lie group corresponding to $span\{I_{j(x,y,z)}\}$ is given by n_j copies of $SU(2)$ (where n_j denotes denotes the number of particles with gyromagnetic ratio γ_j) [4]. Therefore it is isomorphic to $SO(3)$ or $SU(2)$ according to whether n_j is even or odd, respectively.

[4]This is the Lie group of matrices of the form $I_1 \otimes L \otimes I_2$, where the identity matrix I_1 has dimension $2^{n_1 + \cdots n_{j-1}}$, the identity matrix I_2 has dimension $2^{n-n_1-n_2-\cdots n_j}$ and L has dimension 2^{n_j} and is has the form $F \otimes F \otimes \cdots \otimes F$, with $F \in SU(2)$ and the Kronecker product having n_j factors.

5 Lie Algebra Structure and Controllability with Different Gyromagnetic Ratios

In this section, we shall assume that the gyromagnetic ratios $\gamma_1, ..., \gamma_n$ are all different. Therefore we have $r = n$ and, from Lemma 4.1, we have that the control subalgebra $\mathcal{B}$ is the span of the $iI_{j(x,y,z)}$, $j = 1, ..., n$. We shall give a necessary and sufficient condition of controllability and describe the nature of the Lie algebra $\mathcal{L}$, in terms of the properties of the graph $\mathcal{G}\nabla$. This graph will, in general, have a number s of connected components. We first describe the situation when $s = 1$ and then generalize to the case of arbitrary s.

Theorem 2 *Assume we are given a model as in (10), where the values γ_j, $j = 1, \ldots, n$ of the gyromagnetic ratios are all different. If the graph $\mathcal{G}\nabla$ is connected, then*

$$\mathcal{L} = su(2^n). \tag{26}$$

As a consequence the system is operator and state controllable (see Theorem 1).

Proof. We show that all the matrices of the form $iI_{k_1l_1,k_2l_2,...,k_ml_m}$ can be obtained as repeated commutators of A, B_x, B_y, B_z, for every $1 \leq m \leq n$. Lemma 4.1 gives the result for $m = 1$. We first prove that this is true for $m = 2$ as well, and then proceed by induction on m. If $m = 2$, we want to show that we can obtain all the matrices of the form $iI_{kv,lw}$, $k < l$, $v,\ w \in \{x,\ y,\ z\}$. From our assumption on the connectedness of $\mathcal{G}\nabla$, there exists a path joining the node representing the $k-th$ particle and the node representing the $l-$th particle. Let us denote by p the *length* of this path, namely the number of edges between k and l. We proceed by induction on p. If $p = 1$, then at least one among M_{kl}, N_{kl} and P_{kl} is different from zero. If $P_{kl} \neq 0$, we have:

$$[A, iI_{lx}] = i\left(\sum_{h<l}(-N_{hl}I_{hy,lz} + P_{hl}I_{hz,ly}) + \sum_{h>l}(-N_{lh}I_{lz,hy} + P_{lh}I_{ly,hz}),\right) \tag{27}$$

and

$$[[A, iI_{lx}], -iI_{ky}] = -iP_{kl}I_{kxly}. \tag{28}$$

Since $P_{kl} \neq 0$, from the matrix $-iP_{kl}I_{kxly}$, using (repeated) Lie brackets with elements iI_{kf} and/or $iI_{lf'}$, with $f,\ f' \in \{x,\ y,\ z\}$ one can obtain all of the elements of the form $iI_{kv,lw}$, with $v,\ w \in \{x,\ y,\ z\}$. If $P_{kl} = 0$, but $N_{kl} \neq 0$, the same can be proved by taking the commutator with iI_{lx} first and then the commutator with iI_{kz} and analogously, if $N_{kl} = P_{kl} = 0$, by taking the commutator with iI_{ly} first and then with iI_{kz}. Now, assume it is possible to obtain every $iI_{kv,lw}$ for every $k < l$ whose distance is $\leq p - 1$. Let k and l have a path with distance p and let $\bar{l}$ represent a particle/node in between k and l in the path. Let us also assume just for notational convenience that $k < \bar{l} < l$. From the inductive assumption, we know that $iI_{kv,\bar{l}w}$ and $iI_{\bar{l}f,lf'}$ can be obtained for every $v,\ w,\ f,\ f' \in \{x,\ y,\ z\}$. We need to show that we can also obtain every $iI_{kg,lq}$ for every $g,\, q \in \{x,\ y,\ z\}$. Using equation (66) in Appendix A, we get

$$[iI_{kx,\bar{l}x}, -iI_{\bar{l}y,ly}] = iI_{kx,\bar{l}z,ly}, \tag{29}$$

and

$$[iI_{kx,\bar{l}z,ly}, iI_{\bar{l}z,lx}] = \frac{1}{4} iI_{kx,lz}, \tag{30}$$

where we have used the following property of the Pauli matrices

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = \frac{1}{4} I_{2\times 2}. \tag{31}$$

As before, we can now take repeated Lie brackets of the matrix obtained in (30) with matrices of the form iI_{kf} and/or $iI_{lf'}$, with $f,\, f' \in \{x,\ y,\ z\}$, to obtain all of the matrices $iI_{kv,lw}$, for $v,\, w \in \{x,\, y,\, z\}$. This concludes the proof that every Kronecker product with two matrices different from the identity can be obtained, namely $m = 2$ in the above notations.

We now show that every matrix $iI_{k_1 v_1, k_2 v_2, \ldots, k_m v_m}$ can be obtained. Consider the Lie bracket

$$[-iI_{k_1 v_1, k_2 v_2, \ldots, k_{m-1} x}, iI_{k_{m-1} y, k_m v_m}] = iI_{k_1 v_1, k_2 v_2, \ldots, k_{m-1} z, k_m v_m}. \tag{32}$$

Both elements $-iI_{k_1 v_1, k_2 v_2, \ldots, k_{m-1} x}$ and $iI_{k_{m-1} y, k_m v_m}$ are available because of the inductive assumption. If $v_{m-1} = z$, we have concluded otherwise, the Lie bracket with the matrix $iI_{k_{m-1} x}$ or $iI_{k_{m-1} y}$ leads to the desired result. This conclude the proof of the Theorem. □

In the general situation, assume that $\mathcal{G}\nabla$ has s connected components and denote by n_j the number of nodes in the $j-$th component. Set up an ordering of the particles so that the first n_1 are in the first connected component of the graph, the ones from $n_1 + 1$ up to $n_1 + n_2$ are in the second component and so on. We have $n_1 + n_2 + \cdots n_s = n$. The following Theorem describes the structure of the Lie algebra $\mathcal{L}$ in the general case assuming to have different gyromagnetic ratios γ_i, $i = 1, 2, ..., n$.

Theorem 3 *Assume we are given a model as in (10), where the values γ_j, $j = 1, \ldots, n$, of the gyromagnetic ratios are all different. Moreover, assume that the graph $\mathcal{G}\nabla$ has s connected components (as described above), then*

$$\mathcal{L} = \mathcal{S}_1 \oplus \mathcal{S}_2 \oplus \cdots \oplus \mathcal{S}_s, \tag{33}$$

where each $\mathcal{S}_j$, $j = 1, 2, ..., s$ is the subalgebra spanned by the matrices

$$iI_{k_1 v_1, k_2 v_2, \ldots, k_r v_r}, \tag{34}$$

with

$$n_1 + n_2 + \cdots + n_{j-1} < k_1 < k_2 < \cdots < k_r \leq n_1 + n_2 + \cdots + n_j. \tag{35}$$

Proof. First notice that, from equation (64) in Appendix A, it follows immediately:

$$[\mathcal{S}_j, \mathcal{S}_k] = 0, \quad \text{if} \ \ j \neq k. \tag{36}$$

Since the values γ_j are all different, from Lemma 4.1 we have that all the elements of the form iI_{kv}, $k = 1, \ldots, n$, $v \in \{x, y, z\}$, are in $\mathcal{L}$. We can write the matrix A as

$$\begin{array}{rcl} A & = & -i(\sum_{1 \leq k < l \leq n_1}(M_{kl}I_{kxlx} + N_{kl}I_{kyly} + P_{kl}I_{kzlz})+ \\ & + & \sum_{n_1 < k < l \leq n_1+n_2}(M_{kl}I_{kxlx} + N_{kl}I_{kyly} + P_{kl}I_{kzlz})+ \\ & \cdots & + \sum_{n_1+n_2+\cdots n_{s-1} < k < l \leq n}(M_{kl}I_{kxlx} + N_{kl}I_{kyly} + P_{kl}I_{kzlz}), \end{array} \tag{37}$$

using the fact that $M_{kl} = N_{kl} = P_{kl} = 0$ if k and l are in two different connected components. Taking the Lie brackets with elements iI_{kv}, $v \in \{x, y, z\}$, with $n_1 + n_2 + \cdots n_{j-1} < k \leq n_1 + n_2 + \cdots n_j$ (here if $j = 1$, we put $n_0 = 0$), one may show, as in the proof of Theorem 2, that it is possible to obtain all the elements in $\mathcal{S}_j$, $j = 1, 2, ..., s$. Moreover from (36), it follows that these and their linear combinations are the only matrices that can be generated by A, B_x, B_y, B_z. $\square$

Notice that, in the above situation, one may think of the spin system as a parallel connection of s spin systems of dimension n_j, $j = 1 \ldots, s$, controlled in parallel by the same control. The solution of (10) has the form

$$X(t) = \Phi_1(t)\Phi_2(t) \cdots \Phi_s(t), \tag{38}$$

where $\Phi_j(t)$ is the solution of (10) with

$$A = -i \sum_{n_{j-1} < h < k \leq n_j} (M_{hk}I_{hx,kx} + N_{hk}I_{hy,ky} + P_{hk}I_{hz,kz}), \tag{39}$$

and

$$B_v = -i \sum_{k=n_{j-1}+1}^{n_j} \gamma_k I_{kv}, \quad v \in \{x, y, z\}. \tag{40}$$

The controls are the same for every subsystem and the matrices Φ_j in (38) commute due to (36). The set of states that can be obtained with an appropriate control for system (10) is given by the Lie group corresponding to the Lie algebra $\mathcal{L}$ namely, in this case, $SU(2^{n_1}) \otimes SU(2^{n_2}) \otimes \cdots \otimes SU(2^{n_s})$.

Remark 5.1 It is important to notice, and it will be used later in the next Section, that, in Theorems 2 and 3, the assumption of different gyromagnetic ratios is used only to derive that the Lie algebra spanned by $iI_{j(x,y,z)}$ is a subalgebra of $\mathcal{L}$. Thus both statements of Theorems 2 and 3 remain true if, instead of assuming $\gamma_i \neq \gamma_j$ for all $i \neq j$, we assume $span_{j=1,\ldots,n}\{iI_{j(x,y,z)}\} \subseteq \mathcal{L}$. This fact will be used in the following Section.

In the following Theorem, we answer the question of state controllability for spin systems with different gyromagnetic ratio. It follows from Theorem 1 that, if $\mathcal{L} = su(2^n)$, the set of states reachable for system (10) is $SU(2^n)$ and therefore the system is both operator controllable and state controllable in this case. If $\mathcal{L} \neq su(2^n)$,we have seen that the set of states reachable for (10) is $SU(2^{n_1}) \otimes SU(2^{n_2}) \otimes \cdots \otimes SU(2^{n_s})$. To see that the system is not state controllable, notice that the corresponding Lie algebra $\mathcal{L}$ is not *simple* (since each of the subalgebras isomorphic to $su(2^{n_j})$ is actually an ideal in $\mathcal{L}$) and therefore it cannot be isomorphic to $sp(2^{n-1})$ as in Theorem 1, part (3). A more direct and geometric proof of the fact that $SU(2^{n_1}) \otimes SU(2^{n_2}) \otimes \cdots SU(2^{n_s})$ is not transitive on the complex sphere is to reason as follows. Assume for simplicity $s = 2$ and V_1 and V_2 two subspaces, of dimension 2^{n_1} and 2^{n_2} such that the underlying subspace of the overall system is $V_1 \otimes V_2$. Every 'unentangled' state, namely a state of the form $|v_1 > \otimes |v_2 >$, with vectors $|v_1 > \in V_1$ and $|v_2 > \in V_2$ can only be transformed into another unentangled vector $(A \otimes B)(|v_1 > \otimes |v_2 >) = A|v_1 > \otimes B|v_2 >$ and there is no possibility of transforming $|v_1 > \otimes |v_2 >$ into an entangled vector namely a vector that cannot be written as the tensor product of two vectors from V_1 and V_2. On the other hand, entangled states always exist for a pair of non trivial vector spaces V_1 and V_2 (for example, if $|e_j >$, $j = 1, ..., m_1$, is a basis of V_1 and $|f_k >$, $k = 1, ..., m_2$ is a basis of V_2, so that $|e_j > |f_k >$ is a basis of $V_1 \otimes V_2$, consider $\frac{1}{\sqrt{2}}|e_1 > |f_1 > + \frac{1}{\sqrt{2}}|e_{m_1} > |f_{m_2} >$.) We summarize the results in this section with the following theorem.

Theorem 4 *Consider a system of n-spins with different gyromagnetic ratios given by the model (10). For this system all the controllability notions are equivalent and they are verified if and only if the associated graph $\mathcal{G}\nabla$ is connected.*

Remark 5.2 In many physical implementations of the control of spin $\frac{1}{2}$ particles, the z component of the control is held constant. The only changes in the previous treatment occur in the proof of Lemma 4.1. In fact, for this case, one does not have the matrix B_z. However, by using the first one of equations (18), one obtains $-i\sum_{j=1}^{r} \gamma_j^2 \tilde{I}_{jz} \in \mathcal{B}$. Then, using this matrix in place of B_z, one gets all the matrices in (23), (24), (25), with only odd l's in (23), (24), and even l's in (25). If we assume $|\gamma_1| \neq |\gamma_2| \neq \ldots |\gamma_r|$, the result remains unchanged. In fact, the determinant of the matrix referred to at the end of the proof of Lemma 4.1, is still a non zero Vandermonde determinant. The drift matrix A is modified by adding a term $-i\sum_{j=1}^{n} \gamma_j I_{jz} u_z$, with u_z constant but this does not modify the resulting Lie algebra $\mathcal{L}$, since $-i\sum_{j=1}^{n} \gamma_j I_{jz} u_z$ belongs to the control subalgebra.

6 Systems with Possibly Equal Gyromagnetic Ratios

In this section we analyze the graph $\mathcal{G}\nabla$ for networks of spins with possibly equal gyromagnetic ratios and give a sufficient condition of operator controllability for these systems in terms of the properties of this graph. It will follow from the examples in the next section that the equivalence between state controllability and operator controllability, proved in Theorem 4 for systems with different gyromagnetic ratios, does not always hold if we allow two particles to have the same gyromagnetic ratio.

In the following we describe an algorithm on the graph $\mathcal{G}\nabla$ to conclude operator controllability. The main idea and the physical interpretation go as follows. When all the gyromagnetic ratios of the particles are different they 'react' in a different way to the common electro-magnetic field and this 'asymmetry' along with connectedness of the spin network allows us to control all the particles at the same time. However, even if two particles have equal gyromagnetic ratios they might interact in different ways with a third particle which has gyromagnetic ratio different from the two, and this will break once again the symmetry and give controllability.

Let us divide the particles into r sets $S_1^0, ..., S_r^0$ as it was done in Section 3 and assume that at least one set is a singleton, namely, there exists at least one particle which has different γ from all the others. Consider a set $\mathbf{S}$ containing all the singleton nodes. Assuming that there are m of them, let the sets S_1^0,...,S_{r-m}^0 be of cardinality ≥ 2. Now we illustrate a 'disintegration' procedure to divide these sets further.

Algorithm 1

1. Let $\mathcal{C}$ be a collection of sets. Set $\mathcal{C} := S_1^0, S_2^0, ..., S_{r-m}^0$.

2. For each set $\tilde{S}$ in $\mathcal{C}$, consider a particle $\bar{l}$ in $\mathbf{S}$ such that for at least two particles in k and j in $\tilde{S}$
$$\{|M_{k\bar{l}}|, |N_{k\bar{l}}|, |P_{k\bar{l}}|\} \neq \{|M_{j\bar{l}}|, |N_{j\bar{l}}|, |P_{j\bar{l}}|\}. \tag{41}$$
If there is no element in $\mathbf{S}$ and no set in $\mathcal{C}$ having this property STOP. Divide the set $\tilde{S}$ into subsets of particles that have the same value for $\{|M_{k\bar{l}}|, |N_{k\bar{l}}|, |P_{k\bar{l}}|\}$.

3. Consider the sets obtained in Step 2. Put the elements that are in singleton sets in $\mathbf{S}$. If all the elements are in $\mathbf{S}$, STOP.

4. Replace the collection $\mathcal{C}$ with the remaining non singleton sets and go back to Step 2.

We have the following theorem.

Theorem 5 *If Algorithm 1 ends with all the particles in the set* $\mathbf{S}$ *and* $\mathcal{G}\nabla$ *is connected, then the Lie algebra* $\mathcal{L}$ *associated to the spin* $\frac{1}{2}$ *particles system, with* n *particles, is* $su(2^n)$*. As a consequence the system is operator controllable. More in general, if Algorithm 1 ends with all the particles in the set* $\mathbf{S}$ *and* $\mathcal{G}\nabla$ *has* s *connected components of cardinality* n_1, n_2, ..., n_s, $\mathcal{L}$ *is given by (33)-(35) (See Theorem 3).*

Proof. From Remark 5.1, all we have to show is that, in the given situation, the Lie algebra $span_{j=1,...,n}\{iI_{j(x,y,z)}\}$ is a subalgebra of $\mathcal{L}$. Rewrite the drift matrix A as

$$\begin{aligned} A = -i & \sum_{k<l, k\notin S_{r-m}^0, l\notin S_{r-m}^0} (M_{kl}I_{kx,lx} + N_{kl}I_{ky,ly} + P_{kl}I_{kz,lz}) \\ -i & \sum_{k<l, k\in S_{r-m}^0, l\in S_{r-m}^0} (M_{kl}I_{kx,lx} + N_{kl}I_{ky,ly} + P_{kl}I_{kz,lz}) \\ -i & \sum_{k<l, k\in S_{r-m}^0, l\notin S_{r-m}^0} (M_{kl}I_{kx,lx} + N_{kl}I_{ky,ly} + P_{kl}I_{kz,lz}) \\ -i & \sum_{k<l, k\notin S_{r-m}^0, l\in S_{r-m}^0} (M_{kl}I_{kx,lx} + N_{kl}I_{ky,ly} + P_{kl}I_{kz,lz}). \end{aligned} \tag{42}$$

From Lemma 4.1, the matrices $i\tilde{I}_{jv}$, $v \in \{x,\, y\, z\}$ and $j = 1, 2, ..., r$, where r is the number of sets S_j^0, are available to generate the Lie algebra $\mathcal{L}$. In particular, since we have assumed that the last m sets are singletons, the matrices iI_{lv}, $v \in \{x, y, z\}$, $l = n_1 + n_2 + \cdots + n_{r-m}+, ..., n$ are $\in \mathcal{L}$. Now, assume that in the set S_{r-m}^0 there are two elements j and k such that condition (41) is verified for some $\bar{l} \in \mathbf{S}$ and assume, for the sake of concreteness, that the inequality is verified for the P coefficient (minor changes are needed in the other cases). By taking the Lie bracket of A with $i\tilde{I}_{(r-m)x}$, the first term gives zero, since it does not involve any term in the set S_{r-m}^0 (see (64), in Appendix A and the definition of the $\tilde{I}$'s in (11)). The Lie bracket of the second term with $i\tilde{I}_{(r-m)x}$ gives a matrix which is a linear combination of matrices of the form $iI_{kv,pw}$, $k, p \in S_{r-m}^0$ and $v, w \in \{x, y, z\}$. We call this matrix K_{r-m}. Thus, we have

$$
\begin{aligned}
&[A, i\tilde{I}_{(r-m)x}] = K_{r-m}+ \\
&i\left(\sum_{k<l, k\in S_{r-m}^0, l\notin S_{r-m}^0}(-N_{kl}I_{kz,ly} + P_{kl}I_{ky,lz}) + \sum_{k<l, k\notin S_{r-m}^0, l\in S_{r-m}^0}(-N_{kl}I_{ky,lz} + P_{kl}I_{kz,ly})\right).
\end{aligned} \tag{43}
$$

By taking the Lie bracket of (43) with $iI_{\bar{l}y}$, and using Properties 1 and 2 in the Appendix A, we obtain

$$[[A, i\tilde{I}_{(r-m)x}], iI_{\bar{l}y}] = i \sum_{k\in S_{r-m}^0} P_{k\bar{l}} I_{ky,\bar{l}x}. \tag{44}$$

From this matrix, by taking Lie brackets with $i\tilde{I}_{(r-m)v}$ and/or $iI_{\bar{l}v}$, $v \in \{x,\, y\, z\}$, it is possible to obtain all the matrices of the form (44) with all the possible combinations of x, y and z in place of y and x respectively.

Using (63) in Appendix A, it is not difficult to see that

$$[i \sum_{k\in S_{r-m}^0} P_{k\bar{l}} i I_{ky,\bar{l}z}, i \sum_{k\in S_{r-m}^0} P_{k\bar{l}} i I_{kx,\bar{l}z}] = \frac{1}{4} i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^2 I_{kz}. \tag{45}$$

By taking the Lie bracket of this with $-i\sum_{k\in S_{r-m}^0} P_{k\bar{l}} i I_{kx,\bar{l}z}$, we obtain $i\sum_{k\in S_{r-m}^0} P_{k\bar{l}}^3 i I_{ky,\bar{l}z}$ and repeating the calculation as in (45), we obtain

$$[i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^3 i I_{ky,\bar{l}z}, i \sum_{k\in S_{r-m}^0} P_{k\bar{l}} i I_{kx,\bar{l}z}] = \frac{1}{4} i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^4 I_{kz}. \tag{46}$$

Continuing this way, it is possible to obtain all the matrices of the form

$$i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^{2p} I_{kz}, \qquad p = 0, 1, 2, ..., \tag{47}$$

and, with minor changes in the choice of the Lie brackets, we can obtain

$$i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^{2p} I_{kx}, \quad i \sum_{k\in S_{r-m}^0} P_{k\bar{l}}^{2p} I_{ky}, \qquad p = 0, 1, 2, ... \tag{48}$$

Now consider for example, the matrices $i\sum_{k\in S^0_{r-m}} P^{2p}_{k\bar{l}} I_{kz}$ and assume, without loss of generality that the elements $P^{2p}_{k\bar{l}} I_{kz}$ are arranged so that elements that have the same value for P_{kl} appear one after the other in the sum. The associated determinant is (cfr. the proof of Lemma 4.1) a Vandermonde determinant and therefore by appropriate linear combinations we can obtain all the matrices of the form $\sum_{k\in T} I_{kz}$ where T is a generic subset of S^0_{r-m} such that all the values of $|P_{k\bar{l}}|$ are the same, for all the $k \in T$. In particular, if T contains a single element then we place that element in the set of singletons $\mathbf{S}$. The other subsets of S^0_{r-m} are arranged in new sets. It is clear that we can repeat this procedure for the other sets $S^0_1, S^0_2, ..., S^0_{r-m-1}$, and then for the subsets obtained, as described in Algorithm 1. If the procedure ends with all the elements in $\mathbf{S}$ then we have that $span_{j=1,\ldots,n}\{iI_{j(x,y,z)}\}$ is in $\mathcal{L}$ and the Theorem follows from Remark (5.1). □

7 Low dimensional systems

Results on the controllability of spin systems in the cases of $n = 1$ and $n = 2$ particles can be found in [6], [8] and [13]. In this section we consider the model (10) assuming Heisenberg type of interaction namely

$$M_{kl} = N_{kl} = P_{kl} := J_{kl}, \tag{49}$$

for every pair of particles k and l. For this model, in the case $n = 2$, the only noncontrollable case, $\mathcal{L} \neq su(2)$, is when $n = 2$ and the two particles have the same gyromagnetic ratio. In this situation, we have

$$\mathcal{L} = span\{A\} \oplus span\left\{i\left(\sigma_v \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_v\right), \quad v \in \{x, y, z\}\right\}, \tag{50}$$

and the matrix A commutes with all the matrices in $\mathcal{L}$. The Lie algebra $\mathcal{L}$ is isomorphic to $u(2)$.

We treat now completely the case of $n = 3$ interacting spin $\frac{1}{2}$ particles. If the three particles have all different gyromagnetic ratios, then we are in the situation treated in Section 5. There are two more possibilities:

(a) all the three gyromagnetic ratios all equal (i.e. $\gamma_1 = \gamma_2 = \gamma_3$),

(b) two gyromagnetic ratios are equal and the third is different (i.e. $\gamma_1 = \gamma_2$ and $\gamma_1 \neq \gamma_3$, according to the notations in Section 3, we have $S^0_1 = \{1, 2\}$ and $S^0_2 = \{3\}$).

- **case (a)**

This case is particularly simple. In fact, we have:

$$\mathcal{L} = span\{A\} \oplus span\{i\tilde{I}_{1v}, \quad v \in \{x, y, z\}\}, \tag{51}$$

with

$$\left[span\{A\}, span\{i\tilde{I}_{1x}, i\tilde{I}_{1y}, i\tilde{I}_{1z}\}\right] = 0.$$

The Lie algebra $\mathcal{L}$ is isomorphic to $u(2)$ and the model is neither operator controllable nor state controllable from Theorem 1.

- **case (b)**

This situation is more involved and it gives rise to interesting examples. First recall that, from Lemma 4.1, we get, for $v = x, y, z$,

$$\begin{aligned} \mathcal{B}_v &= span\{ -i\,(\sigma_v \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_v) \otimes I_{2\times 2},\ -i(I_{2\times 2} \otimes I_{2\times 2} \otimes \sigma_v)\}, \\ \mathcal{B} &= \mathcal{B}_x \oplus \mathcal{B}_y \oplus \mathcal{B}_z. \end{aligned} \tag{52}$$

To deal with this case, we need to consider three subcases:

(i) $|J_{13}| \neq |J_{23}|$,

(ii) $J_{13} = J_{23}$,

(iii) $J_{13} = -J_{23}$.

For the case (i) we can apply Theorem 5 and conclude that, if the associated graph is connected then $\mathcal{L} = su(8)$ and the system is operator controllable. For the case (ii), the model will turn out to be neither operator controllable nor state controllable. Finally, in the case (iii), the controllability properties of the model will depend on the coefficient J_{12}. In fact the system will be operator controllable (i.e. $\mathcal{L} = su(8)$) if $J_{12} \neq 0$, while, if $J_{12} = 0$, then the system will be state controllable but not operator controllable (so, from Theorem 1, in this case $\mathcal{L}$ is isomorphic to $sp(4)$).

- **case (ii):** $J_{13} = J_{23}$

From a physical point of view, in this case the particles one and two feel the same magnetic field and have the same interaction with the third particle, therefore it is not possible to manipulate separately these two particles. This internal symmetry of the system results in lack of controllability both for the evolution operator and the state. If $J_{13} = J_{23} = 0$, we have:

- if $J_{12} = 0$, then $\mathcal{L} = \mathcal{B}$,
- if $J_{12} \neq 0$, then $\mathcal{L} = span\{A\} \oplus \mathcal{B}$ and the matrix A commutes with all the matrices in $\mathcal{L}$.

Now we consider the case $J_{13} = J_{23} \neq 0$. We first define an operation of 'symmetrization' ρ on the matrices in $u(4)$, as follows:

$$i\rho\,(\sigma_1 \otimes \sigma_2) = i\frac{1}{2}\,(\sigma_1 \otimes \sigma_2 + \sigma_2 \otimes \sigma_1)\,, \tag{53}$$

with $\sigma_1, \sigma_2 \in \{I_{2\times 2}, \sigma_x, \sigma_y, \sigma_z\}$, and we extend ρ to all of the matrices of $u(4)$ by linearity. Let:

$$\mathcal{F}_\rho = \{X \in u(4) \mid \rho(X) = X\}\,. \tag{54}$$

Notice that:

$$X_1, X_2 \in \mathcal{F}_\rho \Rightarrow X_1 X_2 \in \mathcal{F}_\rho. \tag{55}$$

For sake of completeness, we include a proof in Appendix B. Let:

$$\mathcal{H} = \left\{ H = F \otimes \sigma_j \;\middle|\; \begin{array}{l} F \in \mathcal{F}_\rho, \\ \sigma_j \in \{I_{2\times 2}, \sigma_x, \sigma_y, \sigma_z\} \\ H \neq iI_{8\times 8} \end{array} \right\}. \tag{56}$$

First, we have:

$$\mathcal{L} \subseteq \mathcal{H}. \tag{57}$$

To see this, recall that $\mathcal{L}$ is generated by:

$$A = -iJ_{12}\left(\sigma_x \otimes \sigma_x \otimes I_{2\times 2} + \sigma_y \otimes \sigma_y \otimes I_{2\times 2} + \sigma_z \otimes \sigma_z \otimes I_{2\times 2}\right) - iJ_{13}$$

$$\Big((\sigma_x \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_x) \otimes \sigma_x + (\sigma_y \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_y) \otimes \sigma_y + (\sigma_z \otimes I_{2\times 2} + I_{2\times 2} \otimes \sigma_z) \otimes \sigma_z\Big),$$

and by the matrices in $\mathcal{B}$ (see equation (52)). Thus $\mathcal{L} \subseteq \mathcal{H}$ follows from the fact that both A and $\mathcal{B}$ are in $\mathcal{H}$, and that $\mathcal{H}$ is a Lie algebra because of (55). Now we have:

(i) if $J_{12} \neq 0$, then $\mathcal{L} = \mathcal{H}$, and it has dimension 39;

(ii) if $J_{12} = 0$, then $\mathcal{L} \subset \mathcal{H}$, where the inclusion is strict and it has dimension 38.

The proof of both the previous statements (i) and (ii) follows from the analysis of the Lie algebra structure for this model, given in the Appendix C. In both cases $\mathcal{L}$ is not $su(8)$, thus the model is not operator controllable. Moreover, by looking at the two possible dimensions of $\mathcal{L}$, the model can not be state controllable either. In fact to have state controllability we would need, see Theorem 1, $\mathcal{L} = su(8)$ or $\mathcal{L}$ isomorphic to $sp(4)$, which has dimension 36.

- **case (iii):** $J_{13} = -J_{23} \neq 0$

This case is interesting because it provides a physical example of a system which is state controllable but not operator controllable. It also shows that for spin systems with some gyromagnetic ratios possibly equal to each other the two notions of controllability do not coincide (cfr. Theorem 4).

Consider the following vector spaces of matrices

$$\mathcal{M} := span\{iI_{1v,3w} - iI_{2v,3w}, \quad v, w \in \{x, y, z\}\}, \tag{58}$$

$$\tilde{\mathcal{C}} := span\{iI_{1v} + iI_{2v}, iI_{3w}, \quad v, w \in \{x, y, z\}\}, \tag{59}$$

$$\mathcal{N} := span\{iI_{1v,2w,3p} + iI_{1w,2v,3p}, \quad v, w, p \in \{x, y, z\}\}, \tag{60}$$

$$\mathcal{R} := span\{iI_{1v,2w} - iI_{1w,2v}, \quad v \neq w, v, w \in \{x, y, z\}\}. \tag{61}$$

It can be seen by verifying the commutation relations among these vector spaces that $\mathcal{A} := \mathcal{M} \oplus \tilde{\mathcal{C}} \oplus \mathcal{N} \oplus \mathcal{R}$ is a subalgebra. Moreover, using the test in part 4 of Theorem 1, it can be shown that this Lie algebra is isomorphic to $sp(4)$. It is interesting to notice that the decomposition $\mathcal{A} := \mathcal{M} \oplus \tilde{\mathcal{C}} \oplus \mathcal{N} \oplus \mathcal{R}$ is underlying a Cartan decomposition of $sp(4)$ [10] since the following inclusions among the above vector spaces hold:

$$[\tilde{\mathcal{C}} \oplus \mathcal{N}, \tilde{\mathcal{C}} \oplus \mathcal{N}] \subseteq \tilde{\mathcal{C}} \oplus \mathcal{N}, \quad [\tilde{\mathcal{C}} \oplus \mathcal{N}, \mathcal{M} \oplus \mathcal{R}] \subseteq \mathcal{M} \oplus \mathcal{R}, \quad [\mathcal{M} \oplus \mathcal{R}, \mathcal{M} \oplus \mathcal{R}] \subseteq \tilde{\mathcal{C}} \oplus \mathcal{N}. \tag{62}$$

To see that $\mathcal{A}$ is a subalgebra of $\mathcal{L}$ notice that Lemma 4.1 gives a basis for $\tilde{\mathcal{C}}$. By taking the Lie bracket of A with $I_{3x} \in \mathcal{B}$ and then of the resulting matrix with $I_{3z} \in \mathcal{B}$, we obtain a matrix proportional to $i(I_{1z,3x} - I_{2z,3x})$ and, from this, taking Lie brackets with elements in $\tilde{\mathcal{C}}$ we can obtain all the elements in the basis of $\mathcal{M}$ indicated in (58). Thus, both $\tilde{\mathcal{C}}$ and $\mathcal{M}$ are included in $\mathcal{L}$. A basis of $\mathcal{N}$ can be obtained by Lie brackets of appropriate elements of $\mathcal{M}$ (possibly adding an element of $\tilde{\mathcal{C}}$). Finally, a basis of $\mathcal{R}$ can be obtained by Lie brackets of appropriate elements of $\mathcal{M}$ and $\mathcal{N}$. Therefore the Lie algebra $\mathcal{A}$ is a subalgebra of $\mathcal{L}$. The two Lie algebras coincide if $J_{12} = 0$. This is the case remarked above of a system that, according to Theorem 1 is state controllable, since $\mathcal{L}$ is isomorphic to $sp(4)$, but not operator controllable. If $J_{12} \neq 0$, then the matrix A is not in the Lie algebra $\mathcal{A}$. However, it is still possible to generate $\mathcal{A}$, which is isomorphic to $sp(4)$ and, applying part 5 of Theorem 1, we conclude that $\mathcal{L} = su(8)$ in this case, and the system is operator controllable.

The results of this section and Section 6 remain true even if we set $u_z = \textit{constant}$ in the model (10) if we assume that there exist no two values for the gyromagnetic ratios γ_1 and γ_2 such that $\gamma_1 = -\gamma_2$ (cfr. Remark 5.2)

8 Conclusions

We have presented an analysis of the Lie algebra structure associated to a system of n spin $\frac{1}{2}$ particles with different gyromagnetic ratios and inferred its controllability properties. These only depend on the properties of a graph obtained by connecting two nodes representing two particles if the coupling constant between the two particles is different from zero. Controllability of the state and of the unitary evolution operator are equivalent for this class of systems. If the system is not controllable then it is a parallel connection of a number of controllable systems equal to the connected components of the associated graph. The latter result can be easily generalized to the case where the connected components do not represent controllable subsystems, which is a case that might occur if some of the gyromagnetic ratios are equal.

We have given a complete description of the low dimensional cases (up to a number of particles equal to three) with isotropic interaction and possibly equal gyromagnetic ratios. This analysis is of interest since, in many physical situations, a small number of particles is controlled. These results also provide an example of a quantum system which is controllable in the state but not in its unitary evolution operator. Thus, the equivalence of the two notions of controllability, proved for spin systems in the case of different gyromagnetic ratios, is no longer true if some of the gyromagnetic ratios are equal.

This paper also presented a general sufficient condition of controllability for spin systems in terms of the associated graph.

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Appendix A: Some properties of the matrices $I_{k_1l_1,k_2l_2,...,k_rl_r}$

We collect in this appendix some properties of the matrices $I_{k_1l_1,k_2l_2,...,k_rl_r}$, in particular involving the commutators of these matrices. These relations can be easily proven by using the fundamental property:

$$[A \otimes B, C \otimes D] = [A, C] \otimes BD + CA \otimes [B, D], \tag{63}$$

where A and B are square matrices of the same dimensions and B and D are square matrices of the same dimensions as well.

Property 1: If $\{k_1, k_2, ..., k_r\} \cap \{\bar{k}_1, \bar{k}_2, ..., \bar{k}_s\} = \emptyset$ then

$$[I_{k_1l_1,k_2l_2,...,k_rl_r}, I_{\bar{k}_1m_1,\bar{k}_2m_2,...,\bar{k}_sm_s}] = 0, \tag{64}$$

for every possible combination of l_j's and m_j's.

Property 2: Assume that $\bar{k} \in \{k_1, k_2, ..., k_r\}$, and, in particular, $\bar{k} = k_j$.

(a) If $l_j = m$, then

$$[I_{k_1l_1,k_2l_2,...,k_rl_r}, I_{\bar{k},m}] = 0, \tag{65}$$

(b) if $[\sigma_{l_j}, \sigma_m] = \alpha\sigma_\tau$, with $\alpha = \pm i$, then:

$$[I_{k_1l_1,k_2l_2,...,k_rl_r}, I_{\bar{k},m}] = \alpha \, I_{k_1l_1,...,k_j\tau,...,k_rl_r}. \tag{66}$$

Appendix B: Proof of property (55)

In order to see (55), we write any element X of $u(4)$ as follows (we use the definition $\sigma_0 := I_{2\times 2}$ and the ordering $0 < x < y < z$)

$$X = \sum_{j,k=0,x,y,z} \alpha_{jk} i\sigma_j \otimes \sigma_k = \sum_{j=0,x,y,z} \alpha_{jj} i\sigma_j \otimes \sigma_j +$$

$$+ \sum_{j<k} \frac{\alpha_{jk} + \alpha_{kj}}{2} (\sigma_j \otimes \sigma_k + \sigma_k \otimes \sigma_j) + \sum_{j<k} \frac{\alpha_{jk} - \alpha_{kj}}{2} (-\sigma_k \otimes \sigma_j + \sigma_j \otimes \sigma_k).$$

From this expression, it is immediate to see that $X \in \mathcal{F}_\rho$ if and only the terms in the last sum are all zero. Therefore a basis of $\mathcal{F}_\rho$ is given by the matrices of the form

$$i\left(\sigma_l \otimes \sigma_v + \sigma_v \otimes \sigma_l\right), \tag{67}$$

with $l, v = 0, x, y, z$. In view of this fact, it is sufficient to verify (55) on all the matrices of the form (67). This last fact is only a straightforward calculation.

Appendix C: Structure of the Lie algebra $\mathcal{L}$ in the case $n = 3$, $J_{13} = J_{23} \neq 0$ $(\gamma_1 = \gamma_2 \neq \gamma_3)$

We look at the following vector subspaces of $\mathcal{H}$ ($\mathcal{H}$ is the vector space defined in (56).

$$\tilde{\mathcal{C}} := span \quad i\{I_{1v} + I_{2v}, I_{3w} \quad v, w = x, y, z\} \tag{68}$$

$$\mathcal{M} := span \quad i\{I_{1v,3w} + I_{2v,3w} \quad v, w = x, y, z\} \tag{69}$$

$$\mathcal{N} := span \quad i\{I_{1v,2w,3p} + I_{1w,2v,3p} \quad v, p, w = x, y, z\} \tag{70}$$

$$\mathcal{Q} := span \quad i\{I_{1v,2w} + I_{1w,2v} \quad v \neq w = x, y, z\} \tag{71}$$

$$\mathcal{R} := span \quad i\{I_{1x,2x} - I_{1y,2y}, I_{1x,2x} - I_{1z,2z}\} \tag{72}$$

The following commutation relations are easily verified

$$[\tilde{\mathcal{C}}, \tilde{\mathcal{C}}] \subseteq \tilde{\mathcal{C}}, \quad [\tilde{\mathcal{C}}, \mathcal{M}] \subseteq \mathcal{M}, \quad [\tilde{\mathcal{C}}, \mathcal{N}] \subseteq \mathcal{N}, \quad [\tilde{\mathcal{C}}, \mathcal{Q}] \subseteq \mathcal{N} \oplus \mathcal{R}, \quad [\tilde{\mathcal{C}}, \mathcal{R}] \subseteq \mathcal{Q}; \tag{73}$$

$$[\mathcal{M}, \mathcal{M}] \subseteq \tilde{\mathcal{C}} \oplus \mathcal{M} \oplus \mathcal{N}, \quad [\mathcal{M}, \mathcal{N}] \subseteq \mathcal{M} \oplus \mathcal{Q} \oplus \mathcal{R}, \quad [\mathcal{M}, \mathcal{Q}] \subseteq \mathcal{N} \quad [\mathcal{M}, \mathcal{R}] \subseteq \mathcal{N}; \tag{74}$$

$$[\mathcal{N}, \mathcal{N}] \subseteq \tilde{\mathcal{C}} \oplus \mathcal{N}, \quad [\mathcal{N}, \mathcal{Q}] \subseteq \tilde{\mathcal{C}} \oplus \mathcal{M}, \quad [\mathcal{N}, \mathcal{R}] \subseteq \mathcal{M}; \tag{75}$$

$$[\mathcal{Q}, \mathcal{Q}] \subseteq \tilde{\mathcal{C}}, \quad [\mathcal{Q}, \mathcal{R}] \subseteq \tilde{\mathcal{C}}; \tag{76}$$

$$[\mathcal{R}, \mathcal{R}] = 0. \tag{77}$$

A basis of $\tilde{\mathcal{C}}$ is generated by the matrices B_x, B_y, B_z according to Lemma 4.1, while a basis in $\mathcal{M}$ can be obtained calculating the Lie bracket of A with $I_{3x} \in \mathcal{C}$ then taking the Lie bracket with I_{3z} so as to obtain $I_{1z,3x} + I_{2z,3x}$. From this, taking the Lie bracket with elements in $\mathcal{C}$, we can obtain all the elements in the basis of $\mathcal{M}$ in (74). A basis of $\mathcal{N}$ is obtained by Lie brackets of elements in $\mathcal{M}$. In particular, to obtain elements of the form $iI_{1v,2v,3w}$, we calculate $[iI_{1v,3l}+iI_{2v,3l}, -iI_{1v,3p}-iI_{2v,3p}]-\frac{1}{2}iI_{3w}$, with $p \neq l$ $v, p, l \in \{x, y, z\}$ and $i\sigma_w = [\sigma_l, \sigma_p]$. To obtain elements of the form $iI_{1v,2w,3p} + iI_{1w,2v,3p}$, $v \neq w$, $v, w, p \in \{x, y, z\}$, we can calculate Lie brackets of elements of the form $iI_{1m,3m} + iI_{2m,3m}$, with elements of the form $iI_{1n,3n} + iI_{2n,3n}$, with $n \neq m$ and, possibly, calculate the Lie bracket with an element of the form iI_{3l}, $l, m, n \in \{x, y, z\}$. A basis of $\mathcal{Q}$ can be obtained by Lie brackets between elements of the form $iI_{1v,2v,3x} \in \mathcal{N}$ with elements of the form $iI_{1w,3x} + iI_{2w,3x} \in \mathcal{M}$, $v \neq w$, $v, w \in \{x, y, z\}$. A basis of $\mathcal{R}$ can be obtained by the Lie bracket of elements $iI_{1v,2w,3x} + iI_{1w,2v,3x} \in \mathcal{N}$ with elements $iI_{1p,3x} + iI_{2p,3x}$, with $p \neq v \neq w$, $p, v, w \in \{x, y, z\}$.

Notice that if $J_{12} = 0$, then A is an element of the Lie algebra above described $\tilde{\mathcal{C}} \oplus \mathcal{M} \oplus \mathcal{N} \oplus \mathcal{Q} \oplus \mathcal{R}$, while if $J_{12} \neq 0$ we have $\tilde{\mathcal{C}} \oplus \mathcal{M} \oplus \mathcal{N} \oplus \mathcal{Q} \oplus \mathcal{R} = \mathcal{H}/span\{A\}$, and the Lie algebra $\mathcal{L}$, in this case, coincides with $\mathcal{H}$.